



Full wwPDB NMR Structure Validation Report ⓘ

Oct 12, 2020 – 06:01 PM BST

PDB ID : 6YHZ
Title : UvrD helicase RNA polymerase interactions are governed by UvrDs carboxy terminal Tudor domain.
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Deposited on : 2020-03-31

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	FAILED
PANAV	:	FAILED
ShiftChecker	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:477-A:499, A:506-A:532, A:540-A:545 (56)	0.24	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 6 single-model clusters were found.

Cluster number	Models
1	1, 3
2	2, 5
Single-model clusters	4; 6; 7; 8; 9; 10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1143 atoms, of which 572 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription-repair-coupling factor.

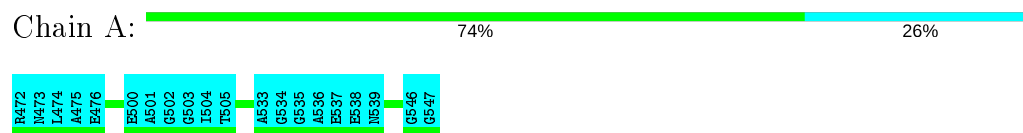
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1143	361	572	101	107	2	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Transcription-repair-coupling factor

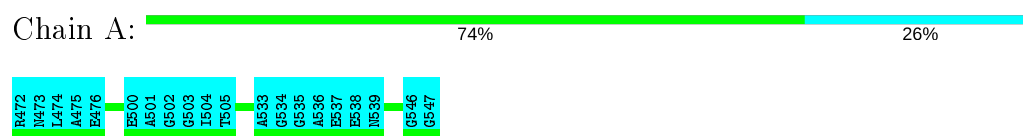


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

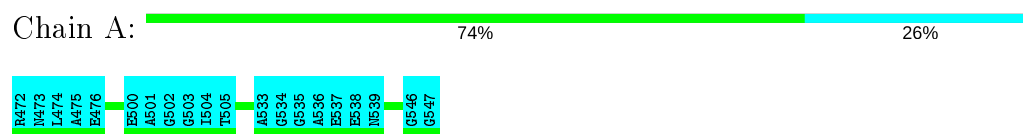
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Transcription-repair-coupling factor



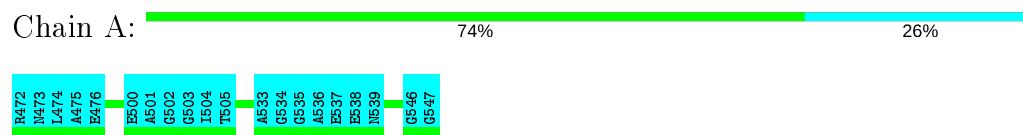
4.2.2 Score per residue for model 2

- Molecule 1: Transcription-repair-coupling factor



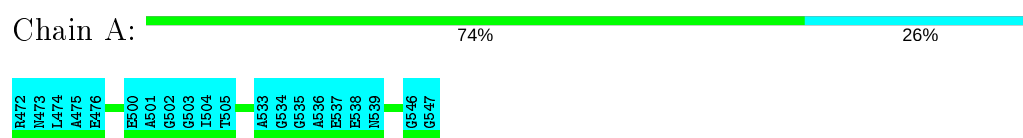
4.2.3 Score per residue for model 3

- Molecule 1: Transcription-repair-coupling factor



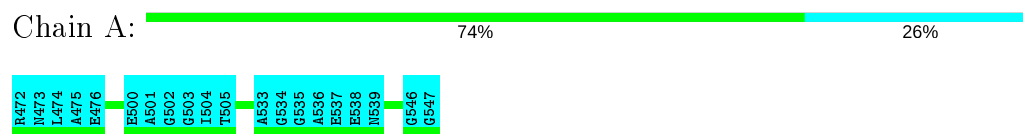
4.2.4 Score per residue for model 4

- Molecule 1: Transcription-repair-coupling factor



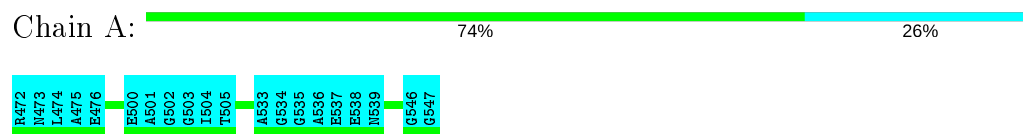
4.2.5 Score per residue for model 5

- Molecule 1: Transcription-repair-coupling factor



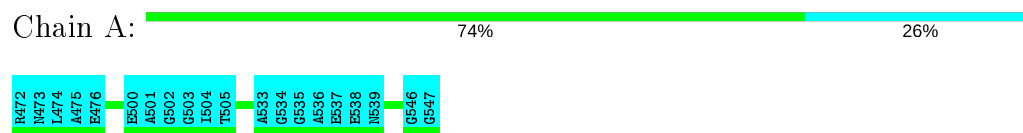
4.2.6 Score per residue for model 6

- Molecule 1: Transcription-repair-coupling factor



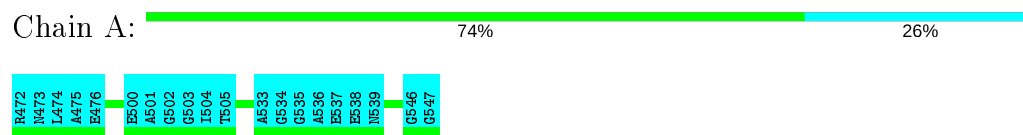
4.2.7 Score per residue for model 7

- Molecule 1: Transcription-repair-coupling factor



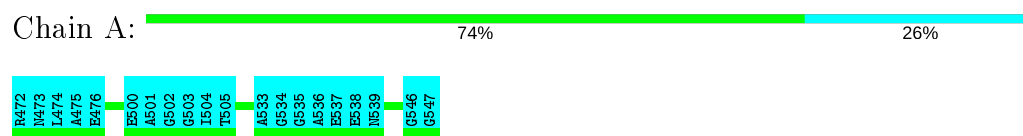
4.2.8 Score per residue for model 8

- Molecule 1: Transcription-repair-coupling factor



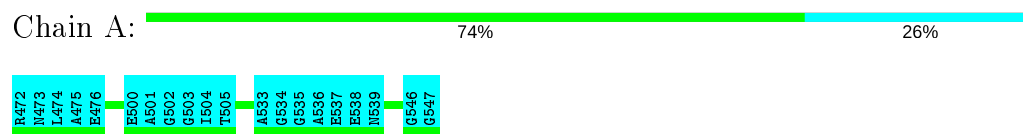
4.2.9 Score per residue for model 9

- Molecule 1: Transcription-repair-coupling factor



4.2.10 Score per residue for model 10

- Molecule 1: Transcription-repair-coupling factor



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *molecular dynamics*.

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *all calculated structures submitted*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	3.98.12
ARIA	refinement	2.3

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

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6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided